Tools and Techniques to Perform Molecular Modelling and Computer-Aided Drug Design

MMTT-2021

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Department of Pharmaceuticals
Ministry of Chemicals & Fertilizers
Government of India

Day 1 Mon, Jan 11	Day 2 Tue, Jan 12	Day 3 Wed, Jan 13	Day 4 Thu, Jan 14	Day 5 Fri, Jan 15	Day 6 Sat, Jan 16	Day 7 Sun, Jan 17
10:00am – 11:15am	09:30am - 11:00am	09:30am - 11:00am	09:30am - 11:15am	09:30am - 11:00am	09:30am - 11:30am	09:30am - 11:30am
	GPSR	**PVB**	**DK / PS**	**NRJ**	**MB**	**JM**
Inaugural Session	Computer-Aided Peptide Therapeutics	CADD in drug metabolism and drug toxicity	Biomolecular Recognition - Insight from Molecular Dynamics Simulations	Use of QM, Docking, and MM methods in Drug Design	Development of Therapeutic Peptides using Machine Learning	Enhanced Sampling Approaches in Biomolecular Simulation
BREAK						
11:30am – 01:00pm	11:15am -12:45pm	11:15am - 01:00pm	11:30am - 01:00pm	11:15am - 01:00pm	11:45am - 01:15pm	11:45am - 01:15pm
GNS	**DP**	**SKD**	**SP**	**HS**	**KR**	**HKS**
Nuts and Bolts of Computer-Aided Drug Design (continues)	Machine Learning Applications for Healthcare	Machine Learning Applications in Predicting Drug-Likeness	Basic Idea of Molecular Modelling and its Application to Improve the Aqueous Solubility of Sparingly Soluble Drugs	Introduction of chemical descriptors and development of machine learning models	Software Tools Developed at the Drug Theoretics & Cheminformatics (DTC) Laboratory	MD Simulations, FEP, and MM-PBSA/GBSA Calculations in Drug Discovery
BREAK						
02:15pm - 03:15pm	02:15pm - 03:15pm	02:15pm - 03:30pm	02:15pm - 05:15pm	02:15pm - 04:15pm	02:15pm - 04:15pm	02:15pm - 05:15pm
HKS Group	**HH**	**SdV**	**ED**	**PB**	**KR Group**	**CC**
Linux, vi, python basics	Computational Exploration of Chemical Reactions and Molecular Interactions	Modelling Enzymatic Reaction Mechanisms	Insights on the Way Acetylcholinesterase is Working	Machine Learning in Cheminformatics	Software Tools Developed at the Drug Theoretics & Cheminformatics (DTC) Laboratory	Modelling of a Membrane Protein with Modeler Membrane Simulation with Desmond
BREAK						
03:30pm - 07:00pm	03:30pm - 07:00pm	03:45pm - 07:15pm	05:30pm - 07:00pm	04:30pm - 07:00pm	04:30pm - 06:30pm	05:15pm - 06:00pm
CG / HKS Group	**MS / SPN**	**GP / HKS Group**	**FAP / TS**	**GNS Group**	**Students' Presentation**	**Valedictory Session**
Gaussian tutorial, Docking and Virtual Screening	Effect of Water-Restructuring Mutations on Ligand Binding to Human Carbonic Anhydrase: A Theoretical Study / Schrodinger	ZASTRA tutorial, Autodock and Gromacs	Applied Molecular Modeling for Drug-Design / Schrodinger	Molecular Property Diagnostic Suite (MPDS)	Evaluation by Experts	MMTT-2021 Team

GNS: Prof. G. Narahari Sastry
GPSR: Prof. G. P. S. Raghava
PVB: Prof. P. V. Bharatam
DK: Prof. Devesh Kumar
NRJ: Dr. Nihar Ranjan Jena
MB: Dr. Manavalan Balachandran
JM: Dr. Jagannath Mondal
PS: Dr. Priyadarshi Satpati
DP: Dr. Deva Priyakumar
SKD: Dr. Sandeep K. Dhanda
SP: Prof. Sandip Paul
HS: Dr. Harinder Singh
KR: Prof. Kunal Roy
HKS: Dr. Hemant K. Srivastava
HH: Prof. Hajime Hirao
SdV: Prof. Sam de-Visser
ED: Prof. Etienne Derat
PB: Dr. Priyanka Banerjee
CC: Dr. Chinmayee Choudhary
MS: Dr. Madhavi Sastry
FAP: Dr. Farhan A. Pasha
SPN: Dr. Sudharsan Pandiyan
TS: Dr. Thomas Steinbrecher
GP: Dr. G. Pillai
CG: Dr. Charitra Gour

Black Color: Invited Talks
Green Color: Hands-on
Purple Color: Invited Talks/Hands-on

Invited Talks are Open to all the Registered Participants and Hands-on Sessions are Restricted to 24 Selected Participants